

2-Methylheptane  
592-27-8 | DTXSID2060460

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 3.99 days

Global applicability domain: Inside

Local applicability domain index: 9.16e-01

Confidence level: 8.64e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2-Methylheptane</div> <div>Measured: 12.5</div> <div>Predicted: 3.99</div>	<div>Image not found</div> <div>2-Methyloctane</div> <div>Measured: 40.7</div> <div>Predicted: 4.23</div>	<div>Image not found</div> <div>3-Methyloctane</div> <div>Measured: 40.7</div> <div>Predicted: 4.08</div>
<div>Image not found</div> <div>4-Methyloctane</div> <div>Measured: 40.7</div> <div>Predicted: 3.58</div>		